

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042018\
 Data File : BF104686.D
 Acq On : 20 Apr 2018 20:34
 Operator : JU/SJ
 Sample : J2460-03
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MDP-B-2-0-6

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	492	498	508	rBV	86848	118193	4.97%	0.499%
2	5.422	562	567	570	rBV	2433760	2306299	97.01%	9.730%
3	6.445	736	741	744	rBV	2370065	2294766	96.52%	9.681%
4	6.575	759	763	766	rBV	2676979	2377472	100.00%	10.030%
5	6.804	798	802	805	rBV	930777	720522	30.31%	3.040%
6	6.957	824	828	832	rBV	2013908	1876764	78.94%	7.918%
7	7.369	893	898	901	rBV	1588763	1408795	59.26%	5.943%
8	8.087	1017	1020	1026	rBV	1098697	906085	38.11%	3.823%
9	9.163	1199	1203	1206	rBV	2786365	2292268	96.42%	9.670%
10	9.239	1212	1216	1218	rVB	43702	40513	1.70%	0.171%
11	9.557	1266	1270	1278	rVB	201446	188185	7.92%	0.794%
12	9.769	1302	1306	1309	rBV	92677	76790	3.23%	0.324%
13	9.845	1315	1319	1323	rBV	978416	905190	38.07%	3.819%
14	10.086	1357	1360	1364	rBV2	27773	26762	1.13%	0.113%
15	10.269	1388	1391	1393	rVB	146167	112887	4.75%	0.476%
16	10.486	1421	1428	1430	rBV	51710	62280	2.62%	0.263%
17	10.633	1450	1453	1464	rVB	1385987	1297616	54.58%	5.474%
18	10.739	1468	1471	1477	rBV	198371	214995	9.04%	0.907%
19	10.933	1501	1504	1508	rBV3	23771	38196	1.61%	0.161%
20	11.186	1544	1547	1550	rBV	174121	156295	6.57%	0.659%
21	11.216	1550	1552	1558	rVB2	74509	84225	3.54%	0.355%
22	11.333	1568	1572	1574	rBV	895741	813331	34.21%	3.431%
23	11.357	1574	1576	1582	rVV	150448	159532	6.71%	0.673%
24	11.404	1582	1584	1587	rVB	32469	30298	1.27%	0.128%
25	11.498	1597	1600	1604	rBV4	23099	27940	1.18%	0.118%
26	11.616	1617	1620	1624	rBV	183066	142766	6.00%	0.602%
27	11.780	1645	1648	1653	rBV5	18057	29542	1.24%	0.125%
28	11.857	1658	1661	1665	rVB3	28164	38780	1.63%	0.164%
29	11.945	1673	1676	1678	rBV3	26568	26612	1.12%	0.112%
30	12.022	1686	1689	1693	rBV	159666	136981	5.76%	0.578%
31	12.310	1735	1738	1740	rBV2	27539	27359	1.15%	0.115%
32	12.410	1752	1755	1763	rVB2	139032	178857	7.52%	0.755%
33	12.545	1775	1778	1783	rBV	270116	228019	9.59%	0.962%
34	12.727	1806	1809	1812	rVB	82583	71267	3.00%	0.301%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.774	1812	1817	1822	rBV2	257377	323272	13.60%	1.364%
36	12.922	1835	1842	1845	rBV	2003491	1910095	80.34%	8.058%
37	12.992	1851	1854	1859	rBV5	20865	31241	1.31%	0.132%
38	13.139	1876	1879	1882	rBV	62017	63571	2.67%	0.268%
39	13.486	1935	1938	1940	rBV	40548	36857	1.55%	0.155%
40	13.774	1983	1987	1991	rBV	110683	142604	6.00%	0.602%
41	13.810	1991	1993	2003	rVB2	134156	179787	7.56%	0.758%
42	13.974	2017	2021	2024	rBV2	656957	703712	29.60%	2.969%
43	14.004	2024	2026	2028	rVB	93602	75632	3.18%	0.319%
44	14.604	2126	2128	2133	rVB2	36367	35303	1.48%	0.149%
45	14.821	2163	2165	2168	rVB	75025	61611	2.59%	0.260%
46	15.021	2196	2199	2202	rBV	76244	97232	4.09%	0.410%
47	15.380	2257	2260	2266	rBV	62570	83359	3.51%	0.352%
48	15.445	2267	2271	2279	rVB2	406355	543270	22.85%	2.292%

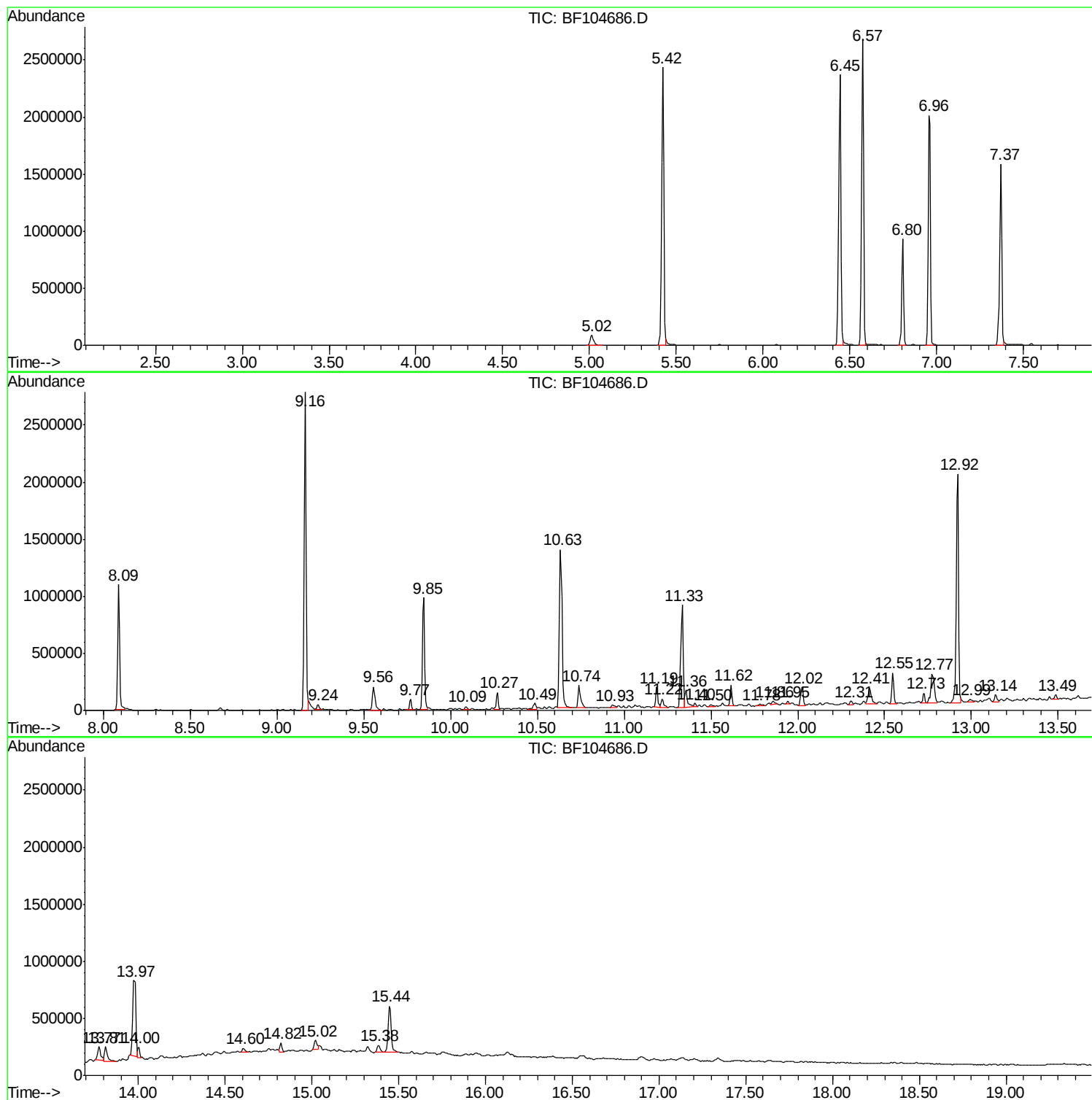
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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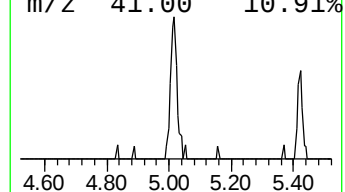
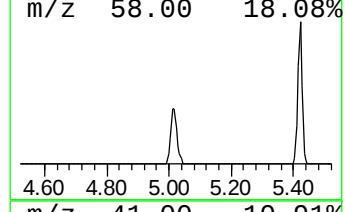
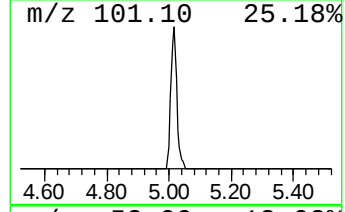
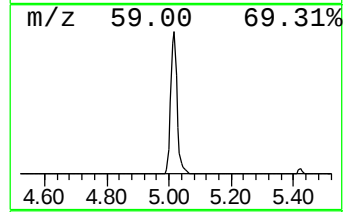
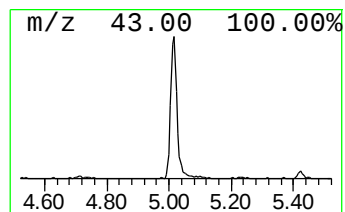
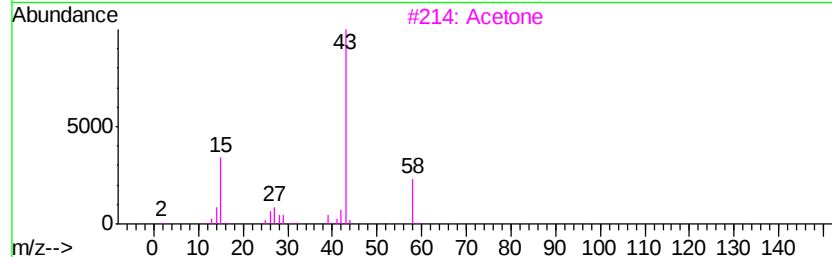
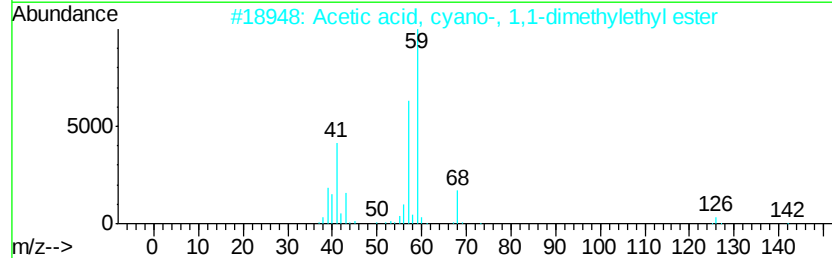
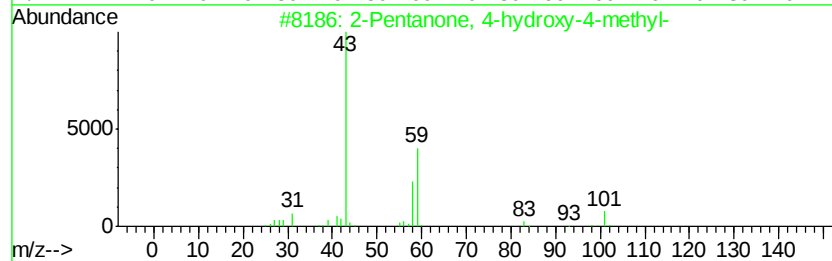
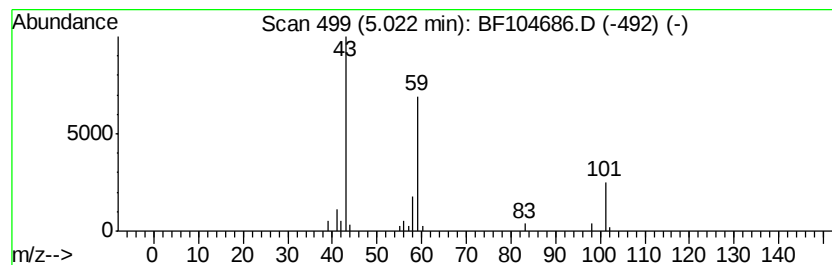
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	3.28 ng	118193	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			Acetone	58	C3H6O	000067-64-1	10
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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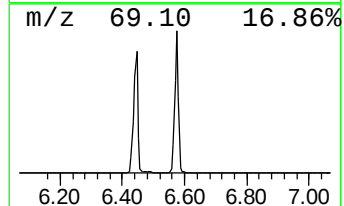
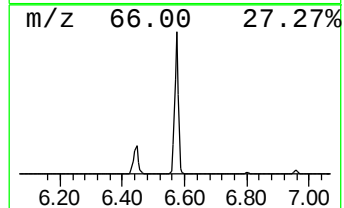
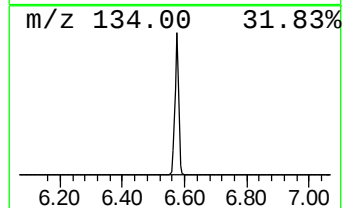
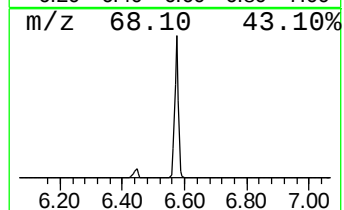
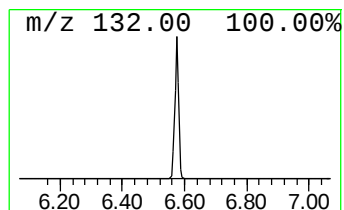
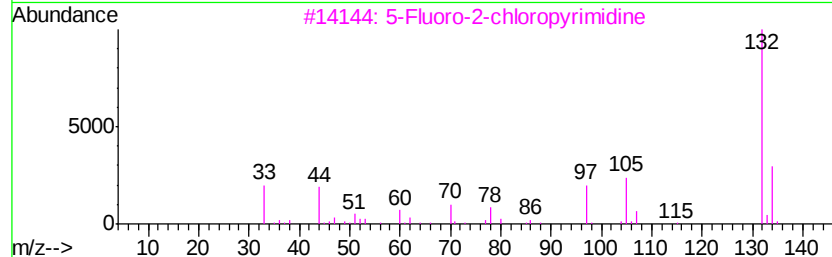
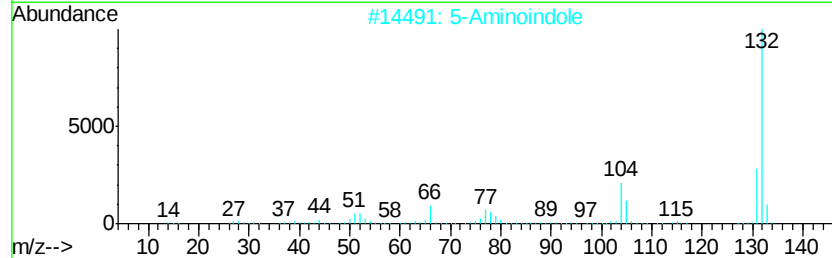
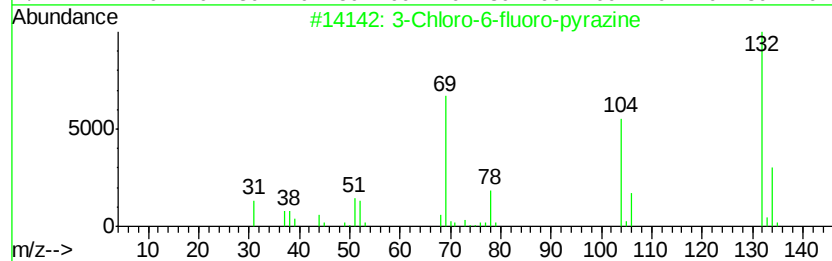
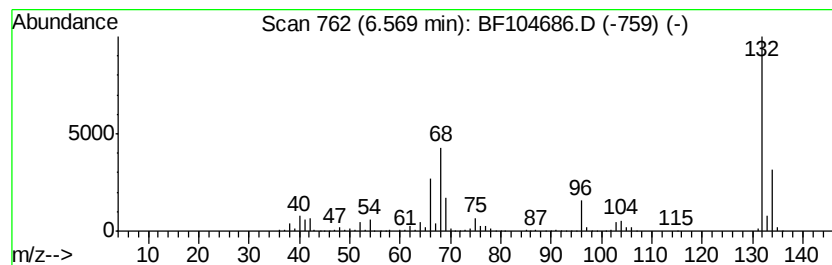
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	65.99 ng	2377470	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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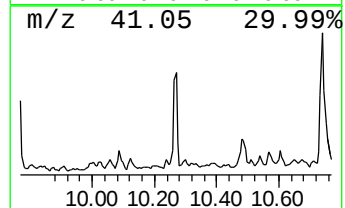
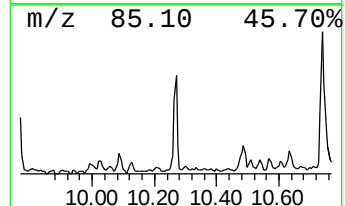
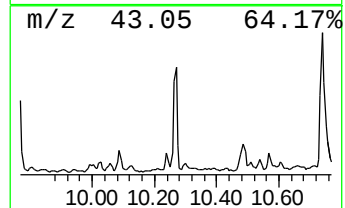
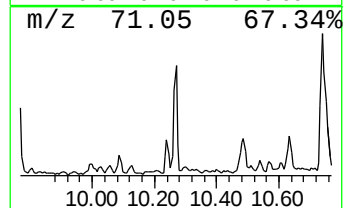
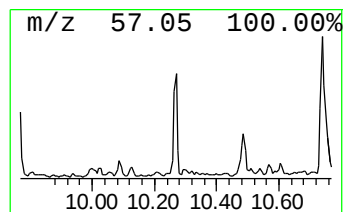
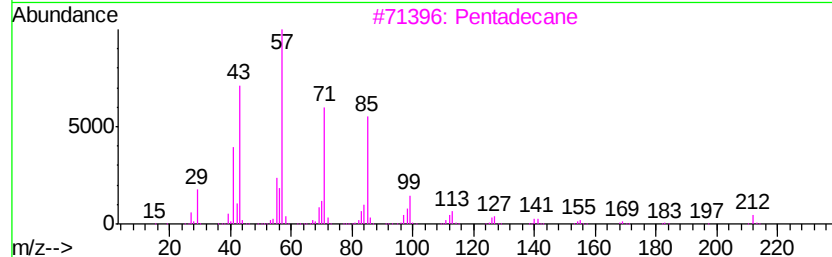
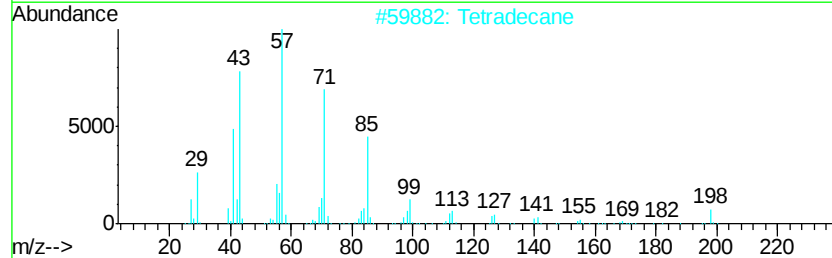
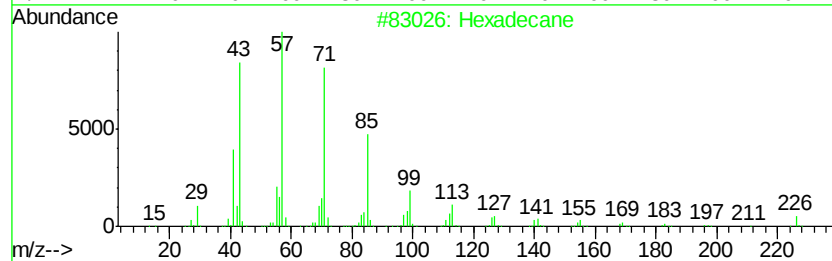
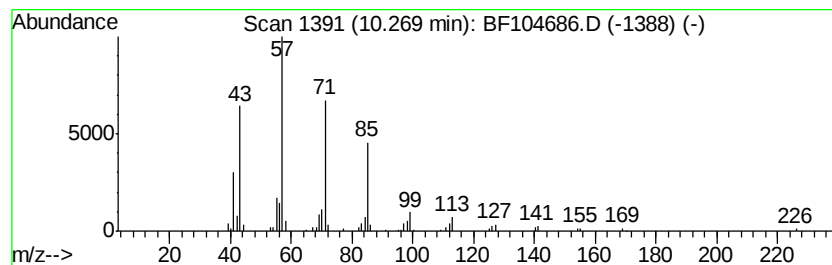
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	2.49 ng	112887	Acenaphthene-d10	9.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	95
2		Tetradecane	198	C14H30	000629-59-4	91
3		Pentadecane	212	C15H32	000629-62-9	91
4		Tridecane	184	C13H28	000629-50-5	90
5		Octacosane	394	C28H58	000630-02-4	86



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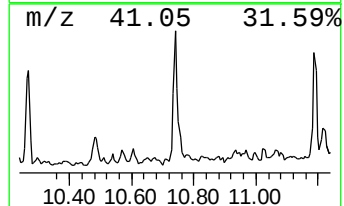
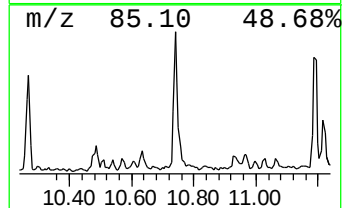
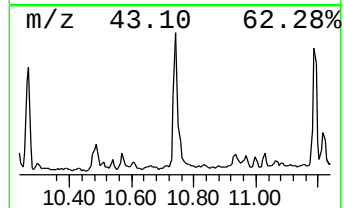
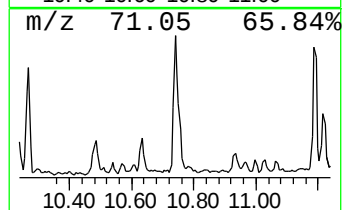
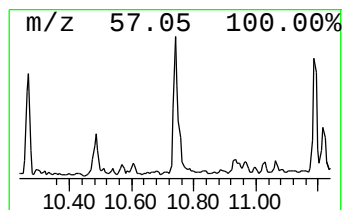
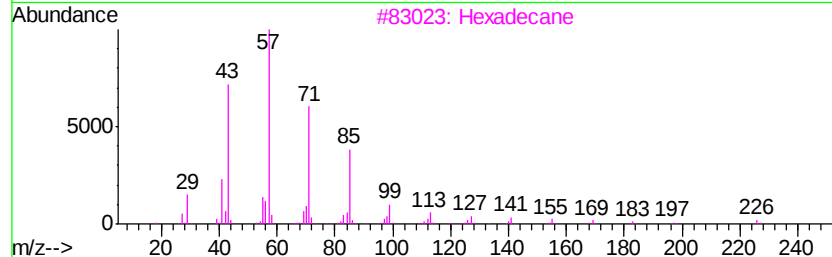
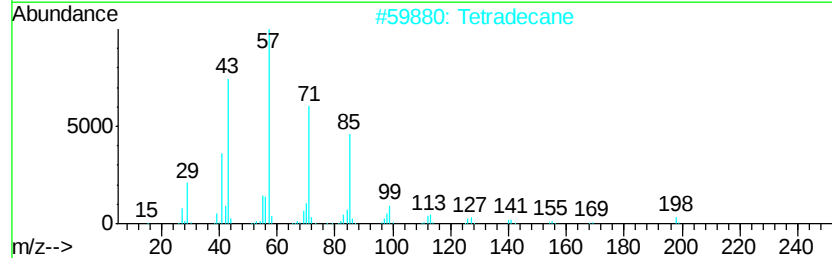
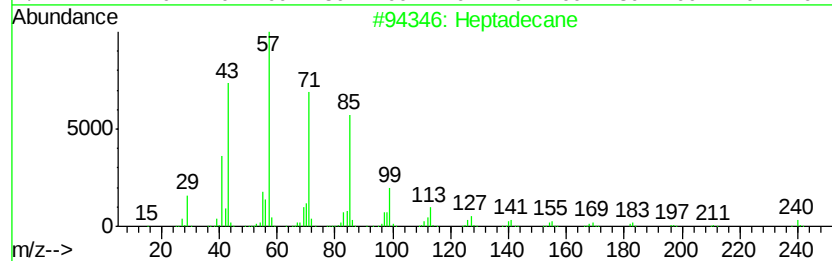
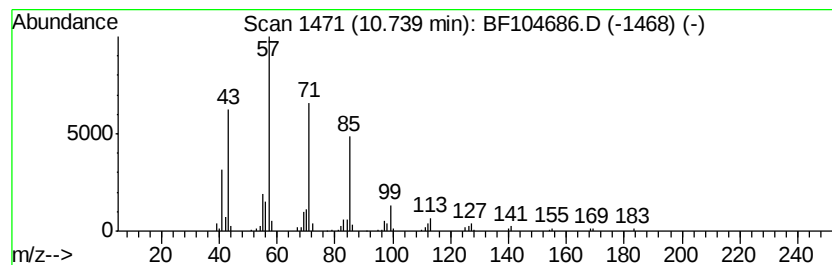
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.74	5.29 ng	214995	Phenanthrene-d10	11.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Tetradecane	198	C14H30	000629-59-4	91
3	Hexadecane	226	C16H34	000544-76-3	90
4	Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	90
5	Tetracosane	338	C24H50	000646-31-1	86



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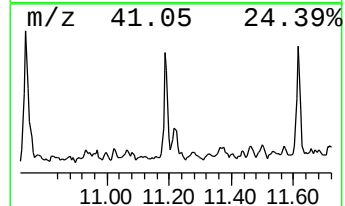
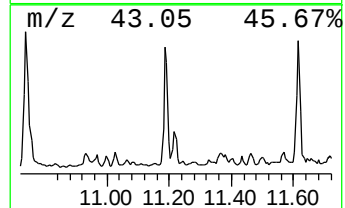
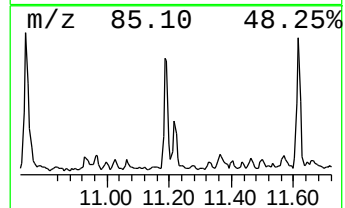
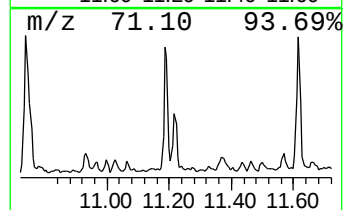
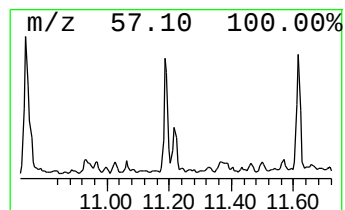
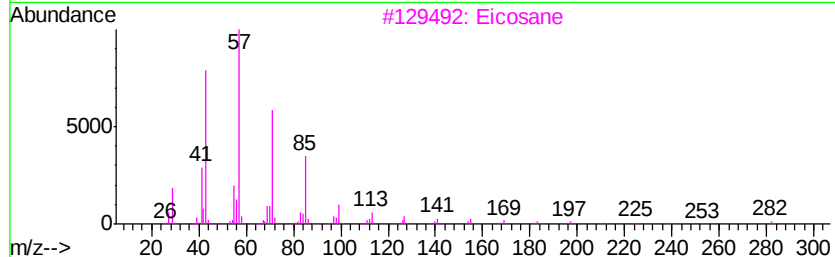
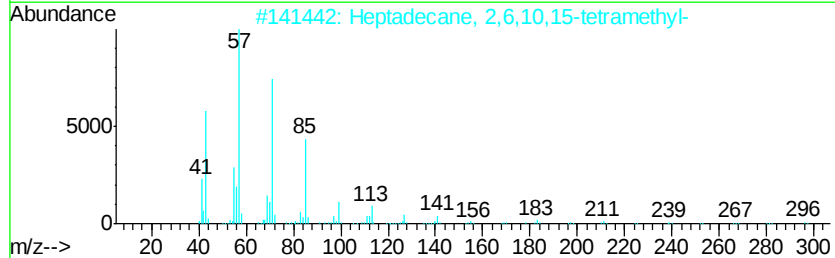
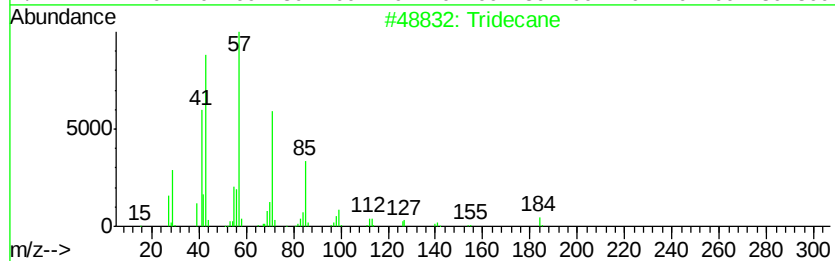
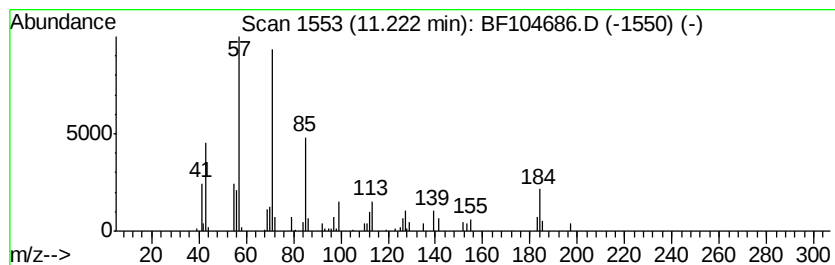
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ClientSampleId :
MDP-B-2-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Tridecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.22	2.07 ng	84225	Phenanthrene-d10	11.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	86
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
3	Eicosane	282	C20H42	000112-95-8	80
4	Heptadecane	240	C17H36	000629-78-7	80
5	Tetracosane	338	C24H50	000646-31-1	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042018\
Data File : BF104686.D
Acq On : 20 Apr 2018 20:34
Operator : JU/SJ
Sample : J2460-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MDP-B-2-0-6

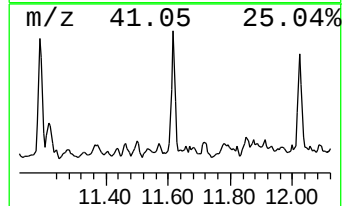
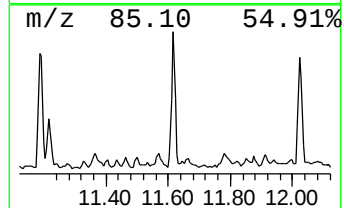
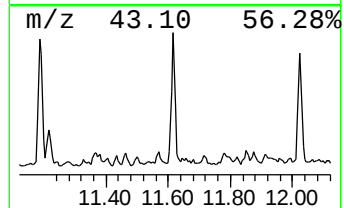
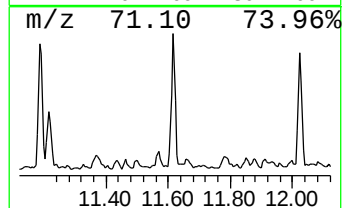
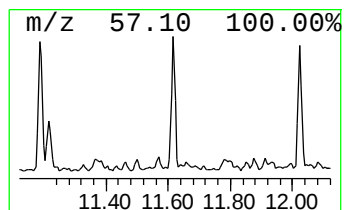
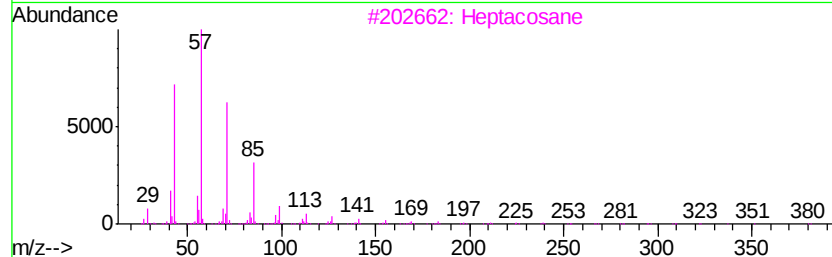
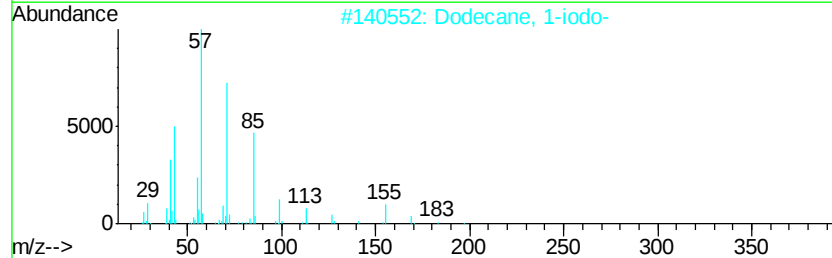
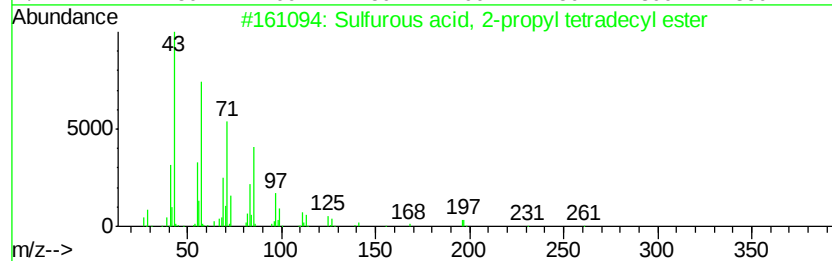
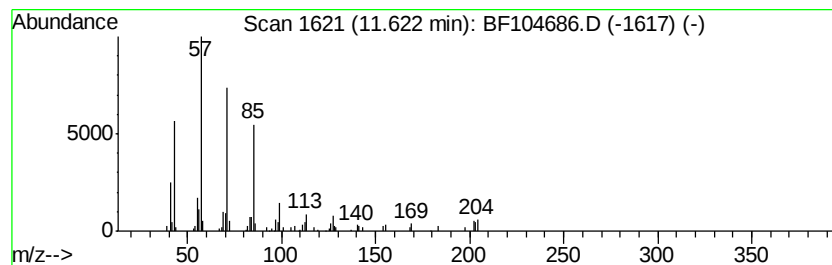
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Sulfurous acid, 2-propyl te... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.62	3.51 ng	142766	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, 2-propyl tetradecyl...	320	C17H36O3S	1000309-12-5	86
2		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
3		Heptacosane	380	C27H56	000593-49-7	83
4		Tetracosane	338	C24H50	000646-31-1	80
5		Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	80



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Sample : J2460-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MDP-B-2-0-6

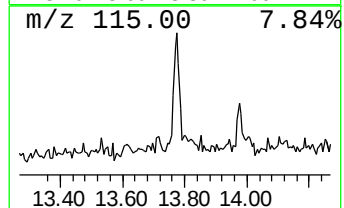
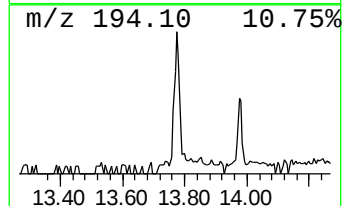
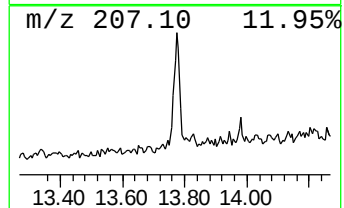
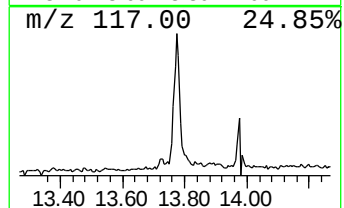
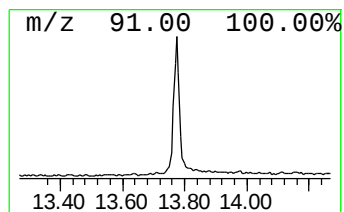
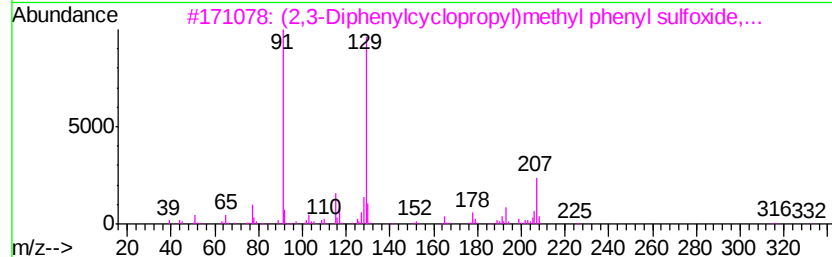
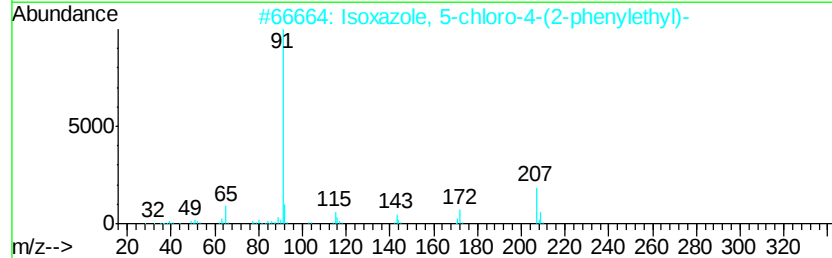
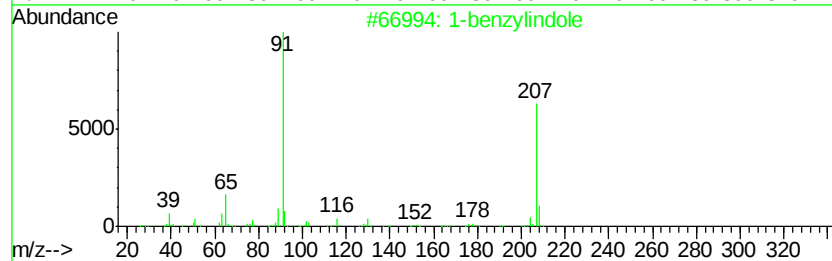
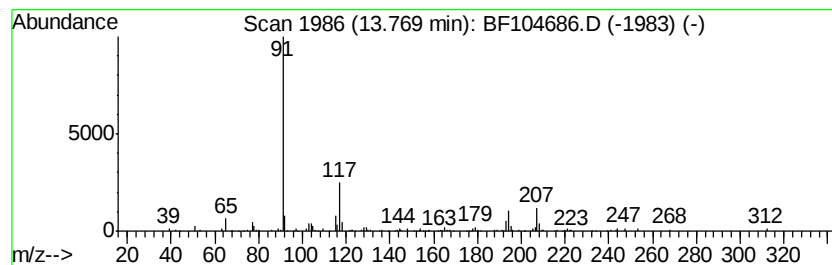
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown13.77 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	4.05 ng	142604	Chrysene-d12	13.98

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-benzylindole	207	C15H13N	1000334-31-3	35
2			Isoxazole, 5-chloro-4-(2-phenyle...	207	C11H10ClNO	1000362-09-0	35
3			(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	25
4			Benzeneacetic acid, phenylmethyl...	226	C15H14O2	000102-16-9	14
5			Ethanone, 2-benzylamino-1-(diben...	340	C23H20N2O	328274-97-1	12



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Sample : J2460-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MDP-B-2-0-6

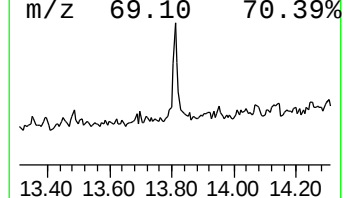
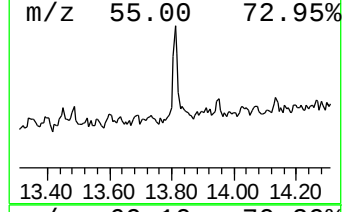
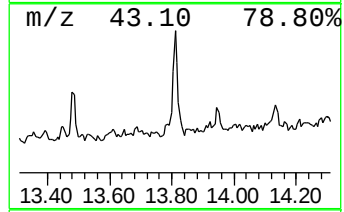
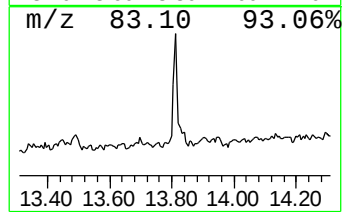
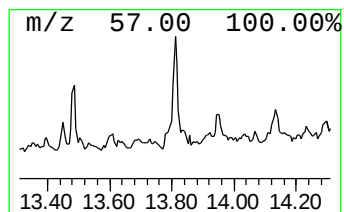
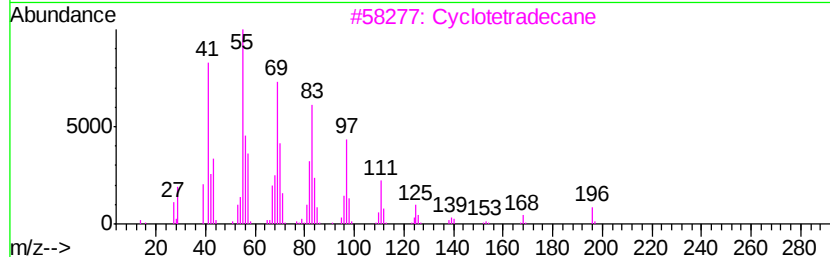
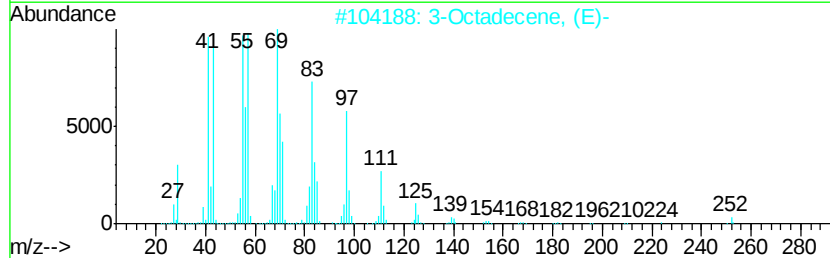
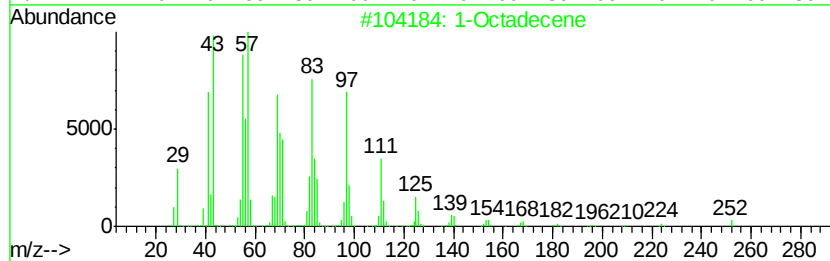
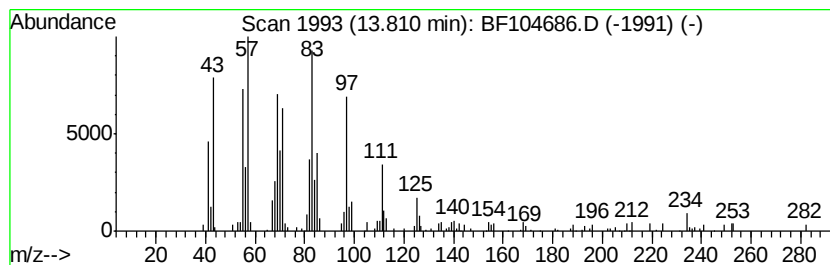
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Peak Number 12 1-Octadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	5.11 ng	179787	Chrysene-d12	13.98

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecene	252	C18H36	000112-88-9	91
2			3-Octadecene, (E)-	252	C18H36	007206-19-1	86
3			Cyclotetradecane	196	C14H28	000295-17-0	83
4			9-Octadecene, (E)-	252	C18H36	007206-25-9	83
5			Octacosanol	410	C28H58O	000557-61-9	83



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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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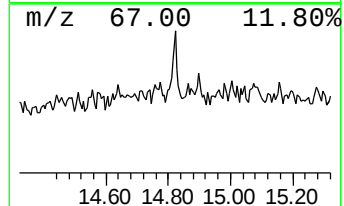
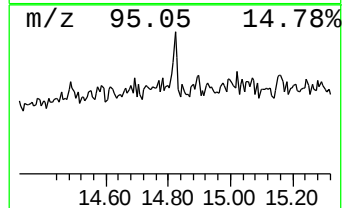
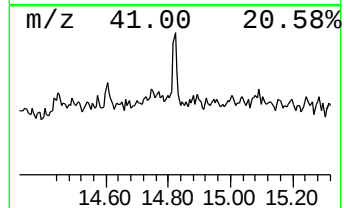
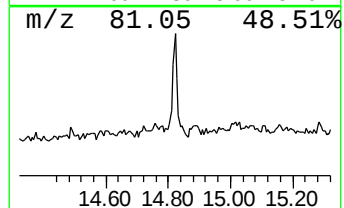
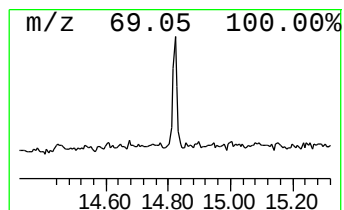
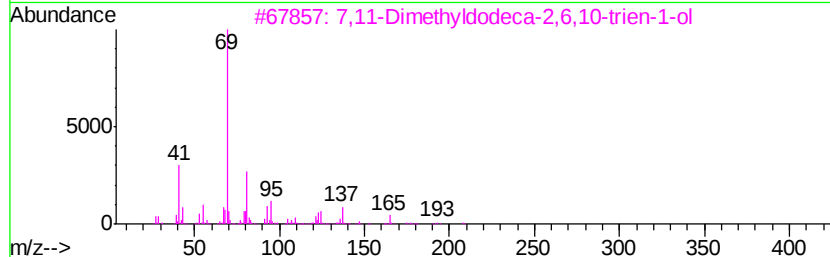
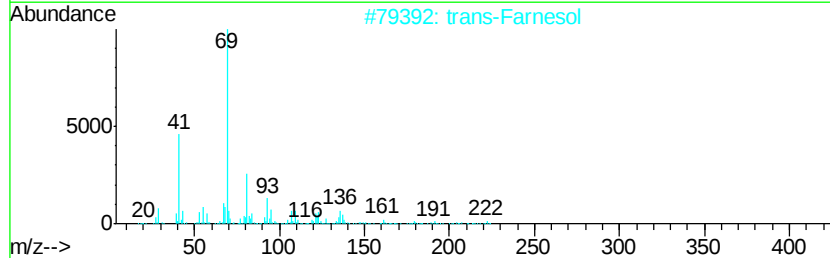
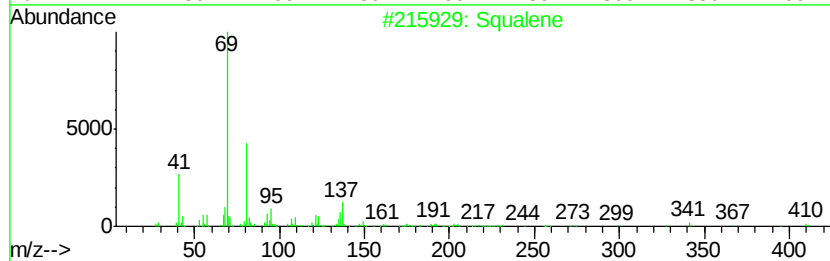
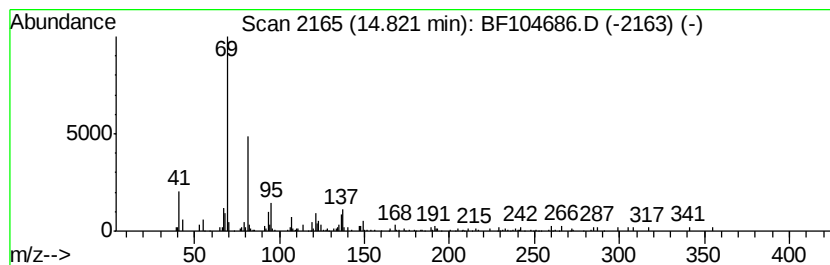
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Peak Number 13 Squalene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	2.27 ng	61611	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	86
2		trans-Farnesol	222	C15H26O	000106-28-5	72
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5		Supraene	410	C30H50	007683-64-9	64



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.57	6.57	66.0	ng	2377470	1	6.80	720522	20.0
Hexadecane	10.27	2.5	ng	112887	3	9.85	905190	20.0
Heptadecane	10.74	5.3	ng	214995	4	11.33	813331	20.0
Tridecane	11.22	2.1	ng	84225	4	11.33	813331	20.0
Sulfurous acid, 2...	11.62	3.5	ng	142766	4	11.33	813331	20.0
unknown13.77	13.77	4.0	ng	142604	5	13.98	703712	20.0
1-Octadecene	13.81	5.1	ng	179787	5	13.98	703712	20.0
Squalene	14.82	2.3	ng	61611	6	15.44	543270	20.0